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METASTABLE SUPERCONDUCTING PAIRS WITH LARGE MOMENTUM

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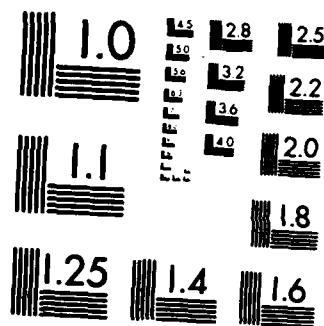
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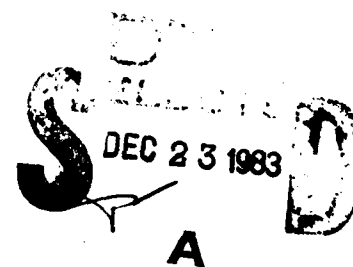
METASTABLE SUPERCONDUCTING PAIRS
WITH LARGE MOMENTUM

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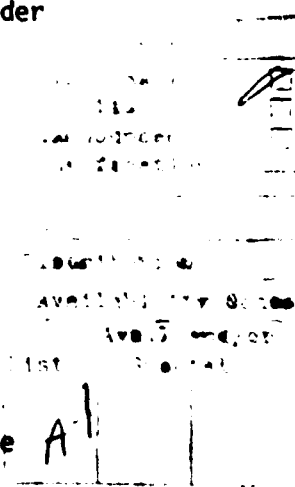
I. Introduction and Statement of Accomplishments

This report summarizes the progress that was made on a theoretical investigation of large momentum pairing in one- and two-dimensional superconductors that was proposed and supported by grant AFOSR-82-0105. The grant period from February 1982 to January 1983 was very productive and extremely successful in that both of the two major objectives of the proposed research were achieved and firm conclusions were obtained. Namely, it was shown that 1) the binding energy of a pair of electrons, in the Cooper model, has a relative maximum at pair momentum greater than $2k_F$, similar to the behavior of a one-dimensional system; and 2) the energy gap and the nature of the ground state were determined for a one-dimensional system when effects of zero momentum pairing, large momentum pairing, and a charge density wave instability are all simultaneously taken into account. The new and significant physics learned from the second objective is that the relative phases of the complex gap parameters for each type of ordering are important. Under suitable conditions, zero momentum pairing, large momentum pairing, and a charge density wave can all coexist.

In the remainder of this report, these two accomplishments are presented in more detail.

II. Binding Energy of a Pair in Two Dimensions

One of the two main objectives of the research was to determine whether the binding energy of a pair of interacting electrons, considered as a function of momentum, has a relative maximum at large momentum or not. During the summer of 1981, Sang Boo Nam, at Wright-



Patterson AFB, and the author showed that for a one-dimensional system the binding energy *does* have a relative maximum at a value of the momentum larger than twice the Fermi momentum. However, for a three-dimensional system, there is *not* such a relative maximum.

As is outlined in the following discussion, we have now shown that the two-dimensional system *does* have a relative maximum in the binding energy at large momentum.

The equation for the binding energy of a pair of electrons is

$$1 = V_{\text{BCS}} \sum_k \frac{1}{(W + \epsilon_1 + \epsilon_2)}$$

where $\epsilon_{1,2} = (q/2 \pm k)^2/2m - k_F^2/2m$, W is the pair binding energy, V_{BCS} is the BCS (Bardeen, Cooper, Schrieffer) coupling constant, q is the total momentum of the pair, k_F is the Fermi momentum describing the density of electrons, and the sum over k is restricted to

$$k_F \leq |q/2 \pm k| \leq K_F \equiv (2m\omega_c + k_F^2)^{1/2}.$$

Here ω_c is the cut-off energy characteristic of the attractive interaction between electrons. It is convenient to deal with the sum over k by treating six separate possibilities, depending on the value of q and ω_c .

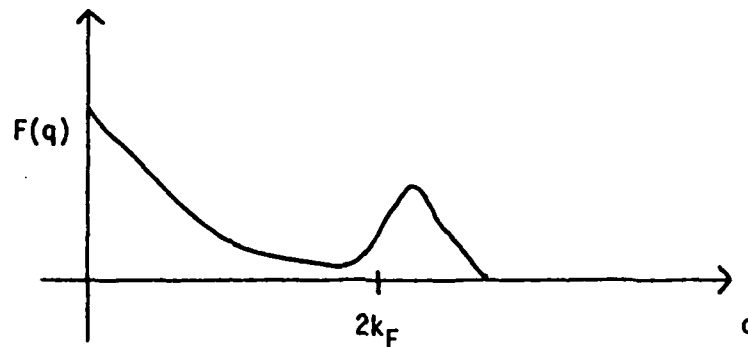
- 1) $q < 2k_F$ and $q < K_F - k_F$
- 2) $q < 2k_F$ and $q > K_F - k_F$
- 3) $q > 2k_F$ and $q < K_F - k_F$
- 4) $q > 2k_F$, $q > K_F - k_F$, and $q < K_F + k_F$
- 5) $q > K_F + k_F$ and $q < 2K_F$
- 6) $q > 2K_F$

It is clear that the sum over k is a monotonically decreasing function of W for fixed q , ω_c , and k_F so that the function $W(q)$ will have maxima

and minima in direct correspondence with the function

$$F(q) = \sum_k \frac{1}{(\epsilon_1 + \epsilon_2)} \quad .$$

$F(q)$ was numerically evaluated and found to have the qualitative behavior shown below for $k_F \geq \frac{1}{3} k_F$.



Thus, in conclusion we were able to show that in a two-dimensional model of a single pair of electrons interacting above an inert Fermi sea, the binding energy may have a relative maximum at values of momentum greater than $2k_F$.

III. Stability of the One-Dimensional System

The second major objective of the research was to determine how metastable large momentum pairs affect the one-dimensional superconductor. As was indicated in the introduction, it was found that when zero momentum pairing, finite momentum pairing, and the Peierls transition charge density wave distortion are all taken into consideration, all three types of order may occur, and their relative phases are important. A brief discussion of the physics follows.

The Hamiltonian of the system is assumed to be

$$H = \sum_k \epsilon_k c_{k\sigma}^+ c_{k\sigma} - \sum_{\substack{k, k', q \\ \sigma, \sigma'}} \frac{V_{kk'q}}{2} c_{k+q\sigma}^+ c_{k'\sigma'}^+ c_{k'+q\sigma'} c_{k\sigma}$$

where the c^+ 's and c 's are the usual electron creation and destruction operators, ϵ_k is the free-particle kinetic energy, and $V_{kk'q}$ denotes the matrix elements for two electron scattering. In a mean-field approximation, the second term is simplified by introducing the fields

$$\Delta_0 e^{i\phi_0} = \sum_k V_0 \langle c_{-k\uparrow}^+ c_{k\uparrow} \rangle \quad ,$$

$$\Delta_Q e^{i\phi_2} = \sum_k 2V_Q \langle c_{Q-k\uparrow}^+ c_{k\uparrow} \rangle \quad ,$$

$$\Delta_Q e^{i\phi_2} = \sum_k 2V_Q \langle c_{-k\uparrow}^+ c_{k-Q\uparrow} \rangle \quad ,$$

$$\Delta_{CDW} e^{i\phi_{CDW}} = \sum_k V_{CDW} [\langle c_{k-Q\uparrow}^+ c_{k\uparrow} \rangle + \langle c_{-k\uparrow}^+ c_{Q-k\uparrow} \rangle] \quad .$$

Here the coupling constants V_0 , V_Q , and V_{CDW} are determined by the values of the interaction matrix elements $V_{kk'q}$, and the four operator term in the Hamiltonian is approximated by using

$$\begin{aligned} c_1 c_2 c_3 c_4 &\approx \langle c_1 c_2 \rangle c_3 c_4 + \langle c_3 c_4 \rangle c_1 c_2 - \langle c_1 c_2 \rangle \langle c_3 c_4 \rangle \\ &\quad - \langle c_1 c_3 \rangle c_2 c_4 - \langle c_2 c_4 \rangle c_1 c_3 + \langle c_1 c_3 \rangle \langle c_2 c_4 \rangle \\ &\quad + \langle c_1 c_4 \rangle c_2 c_3 + \langle c_2 c_3 \rangle c_1 c_4 - \langle c_1 c_4 \rangle \langle c_2 c_3 \rangle \end{aligned}$$

The Hamiltonian is now reduced to only terms containing two c operators and can be diagonalized if we assume the momentum of the CDW and the finite momentum pairing are the same, namely, Q . The resulting energy

eigenvalues depend crucially on the function

$$g = \Delta_Q^2 \{ \Delta_0^2 \cos^2 x + \Delta_{CDW}^2 \sin^2 y \} \\ + [\epsilon_k + \epsilon_{k-Q}] \Delta_0 \Delta_Q \Delta_{CDW} \cos x \cos y$$

where x and y are given by the phases of the mean fields:

$$x = \phi_0 - \frac{1}{2} (\phi_1 + \phi_2)$$

$$y = \phi_{CDW} - \frac{1}{2} (\phi_1 - \phi_2)$$

The most stable state occurs when x is an integer multiple of π and y is an odd multiple of $\pi/2$. For example, $\phi_0 = 0$, $\phi_1 = \pi/2$, $\phi_2 = 3\pi/2$, $\phi_{CDW} = \pi$ produces a stable configuration, and the relative phases of the different types of order are seen to be significant.

Finally, we also note that the values of the coupling constants V_0 , V_Q , and V_{CDW} are of primary importance in determining which fields are non-zero. Essentially the required result for Δ_Q to be finite is that $V_Q \geq V_0$.

IV. Publications

So far, the results of this research have not been published, although two manuscripts have been written. One of these is a collaborative effort with Sang Boo Nam at Wright Patterson AFB and the other was prepared totally by Nam. It is expected that both papers will be published in the future.

V. Personnel

The research described here was pursued at Kent State University by the principal investigator, D.W. Allender, and by an undergraduate student, Beth Cunningham, who carried out some of the numerical computations as part of a senior year individual investigation project. Beth received her B.S. in May 1982.

VI. Interactions

The primary interaction supported by this grant was the collaboration between the principal investigator and S.B. Nam at Wright-Patterson AFB. Two trips were made to Wright-Patterson AFB, one in June 1982 and the other in August 1982. Fruitful discussions were held, also involving D.C. Reynolds.

Also supported was a presentation at the March 1982 meeting of the American Physical Society in Dallas, Texas, entitled "Finite Momentum Pair State in One Dimension" and published in abstract form in Bull. Am. Phys. Soc. 27, 156 (1982).

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20. (cont.)

effective interaction coupling constants. For the two-dimensional system, it was shown that analogous to previously known results in one dimension, the binding energy of electron pairs, as a function of momentum, has a relative maximum at momentum greater than twice the Fermi momentum.



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